

Thermochemical and Fluid Dynamic Model of a Bench-Scale Torrefaction Reactor

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Abstract In biomass-to-energy systems, torrefaction represent an interesting pre-treatment, as it increases the feedstock energy content and its suitability for the subsequent thermal conversion process. The aim of this work is to develop and validate a numerical model for the torrefaction of common reed (*Phragmites australis*). In order to predict the rate of the biomass decomposition (i.e., yield of the reaction products) and characterise the thermofluid-dynamics of the reactor, a heat, mass and momentum transfer model based on a finite volumes method (f.v.m.) representation has been developed and supplemented with a torrefaction kinetic model, consisting of a two-step scheme previously proposed. The kinetic model has been calibrated utilizing the results of thermogravimetric analysis applied to common reeds. Experimental tests have been also performed on reeds in a bench-scale batch apparatus, varying the main process parameters. The validation of the proposed kinetic scheme has been carried out following two different approaches. Through the first (simplified) approach, the finite elements model has been used to estimate the temperature distribution inside the reactor during the experimental tests. An average (experimental) torrefaction temperature has been then calculated and used as input of the kinetic model. In the second approach, the proposed kinetic scheme has been implemented directly in the f.v.m. model, solving numerically the mass and energy conservation equation. The results

obtained by means of the two modelling approaches have been then compared with the experimental data. The proposed thermochemical and fluid dynamic model seems to be a suitable tool for the simulation of a torrefaction reactor and useful for the characterisation and optimization of such kind of systems.

Keywords Thermofluidynamic · Numerical modelling · Torrefaction · Common reed

Abbreviations

a	Thermal diffusivity ($\text{m}^2 \text{s}^{-1}$)
α	Convective heat transfer coefficient ($\text{W m}^{-2} \text{K}^{-1}$)
ϕ	Porosity (–)
μ	Dynamic viscosity ($\text{kg s}^{-1} \text{m}^{-1}$)
ρ	Density (kg m^{-3})
$\bar{\tau}$	Stress tensor (Pa)
c_p	Specific heat ($\text{J kg}^{-1} \text{K}^{-1}$)
E	Specific energy (J kg^{-1})
E_a	Activation energy (J mol^{-1})
$\vec{v}$	Overall velocity vector (m s^{-1})
p	Static pressure (Pa)
$\vec{F}$	External body forces (N)
$\vec{g}$	Gravitational acceleration (m s^{-2})
h	Sensible enthalpy (J kg^{-1})
h_{tor}	Heat required for torrefaction (J kg^{-1})
I	Unit tensor (–)
k	Thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)
k	Reaction rate (s^{-1})
k_0	Pre-exponential factor (s^{-1})
q	Heat flux (W m^{-2})
R	Universal gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)
S_h	Heat source (W m^{-3})
T	Temperature (K)

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Introduction

Most of the solid biomass traditionally used as fuel for heating purposes (e.g., woodchips, wood pellets, cordwood) were products or by-products of forests management and timber industry. An innovative vision looks at developing energy chains consisting of a sequence of treatments, converting the biomass into gaseous or liquid fuels that can be used in a more efficient way. In this frame, a possible biomass pre-treatment is torrefaction. It can be considered as a slow pyrolysis process carried out at low temperatures (max. 280–300 °C) that enhances physical and thermochemical properties of biomass [1–6]—such as grindability, uniformity, hydrophobicity and heating value—and can be a suitable pre-treatment to improve gasification of the feedstock, as well as combustion or co-combustion in existing power plants [7].

Regarding kinetics of torrefaction some models are available in the literature. Investigating the thermal degradation of xylan, Di Blasi and Lanzetta [8] have assumed a two-step mechanism involving the formation of an intermediate solid compound having a reduced degree of polymerization. This intermediate then reacts to give the final product. Prins [9, 10] has proposed that the weight mass loss of willow wood during torrefaction treatment can be described by a similar two-step mechanism. The model of Rousset et al. [11] assumes that wood thermal decomposition can be represented by the decomposition of its main constituents (lignin, cellulose and hemicellulose) according to their amounts in the wood. Lignin decomposes into char and volatiles through a single step path, while cellulose decomposes independently into tar and char plus volatiles, according to the Broido–Shafizadeh model [12, 13]. The decomposition of hemicellulose has been modelled by means of the above mentioned Di Blasi and Lanzetta scheme [8]. For a detailed description of torrefaction kinetics and mechanism it is worth to refer also to [14].

A chemical-physical model for biomass torrefaction reactors has been developed by Ratte et al. [15] coupling two systems, the particle and the surrounding gas system. This model is able to predict composition, temperature and pressure profiles inside a biomass particle and in the surrounding convective gas in different position in the reactor and at different times. The model supplements the kinetics solver based on [16], with a heat, mass and momentum transfer solver based also on the Whitaker model [17] for the drying process and based on Ratte et al. model [18] for thermal degradation.

Most of the presented models mainly focus on the reaction kinetics, giving a zero-dimensional description of the torrefaction process at a micro-particle scale [9–13], or describe the heat, mass and momentum transfer at the

particle scale [15, 18] without considering the 3-dimensional fluid dynamics effects inside the reactor.

The aim of this work is to develop and validate a torrefaction model based on a comprehensive approach consisting of a 3-dimensional thermofluidynamic representation of an experimental torrefaction reactor supplemented with a two-step kinetic scheme previously proposed [9, 10]. The kinetic model has been validated versus TGA data, while the heat, mass and momentum transfer model has been tested using the experimental results of a lab scale batch reactor for biomass torrefaction. Furthermore, the biomass thermal properties have been measured through laser flash analysis method. These parameters are of great importance in numerical modelling, being related to the sensitivity of the model predictions [19, 20].

Among the different species of grass biomass, common reeds (*Phragmites australis*) have been chosen. In fact, growing crops (both herbaceous and woody) have gained widespread appeal for energy production in the last years [21]. Reed is one of the most common plants living in wet ecosystems [22] and can play an important role as local energy source in places where it is naturally present in great amounts [23]. In addition, wetland plants have a high macronutrients accumulation capability because of their generally fast growth and high biomass production [24]. As a consequence, their utilization for energy production could have, as additional advantage, the disposal of such kind of elements from the ecosystem.

Materials and Methods

Thermal Analysis

The thermal behaviour of reeds has been characterized using a simultaneous thermogravimetric analyser (STA 449F3, Netzsch). This technique combines both the heat flux differential scanning calorimetry (DSC) and thermogravimetry (TG). STA analyses were performed at a constant heating rate of 20 °C min^{−1} under inert nitrogen atmosphere in a temperature range from 30 to 1,000 °C. Additional tests have been carried out setting an intermediate temperature plateau at 250 °C in order to assess the effect of a possible torrefaction stage and increase the experimental data suitable for the calibration of the torrefaction kinetic model.

Reed tissues have been ground with a Retsch Mill MM400 in order to obtain particles of less than 0.25 mm size. The powder has been compressed in a steel press, in order to obtain a round tablet of 12.64 mm diameter and 2.00 mm thickness, with a density of 0.87 g cm^{−3} (sample dried at 65 °C for 48 h). The thermal properties (i.e., thermal diffusivity, specific heat and thermal conductivity)

of the so obtained reed disk have been determined experimentally through laser flash analysis (LFA) method in a NETZSCH LFA 447 NanoFlash apparatus; in this method, the front side of a plane-parallel sample is heated by a short light pulse, provided by an high-power Xenon flash lamp, surrounded by a parabolic mirror (reflector) and able to supply a radiant pulse energy up to 10 J in the wavelength range of 150–2,000 nm. The energy pulse length can be adjusted to 0.1, 0.2 or 0.4×10^{-3} s. The resulting temperature rise on the rear surface is measured using an infrared detector. In particular, the LFA 447 uses an InSb-IR detector in the wave-length range of 2,000–5,000 nm cooled by liquid nitrogen; this allows a rapid non-contact measurement of the temperature rise in the back of the sample. By analysis of the resulting temperature-versus-time curve with the Cowan method [25, 26], the thermal diffusivity has been determined at different temperatures (every 25 °C in the range 25–175 °C, three repetitions for each measurement). The upper limit for thermal diffusivity measurement has been chosen in order to avoid any gaseous products release. In fact, products condense on colder areas of the system (e.g., on the protection windows between furnace and IR detector) would cause measurement errors. As far as the validity of this kind of measurement is regarded, the LFA 447 is capable of thermal diffusivity measurements in the range of 0.01 – $1,000 \text{ mm}^2 \text{ s}^{-1}$, with an accuracy of 3–5 % for most materials.

The specific heat (c_p) of reed has been also determined, performing an additional measurement with a reference graphite sample of known c_p . In fact, under the same measurement conditions, the heat provided to the sample and to the reference is the same, which lead to the following equation:

$$c_{p,\text{sample}} = \frac{m_{\text{ref}}}{m_{\text{sample}}} \cdot \frac{\Delta T_{\text{ref}}}{\Delta T_{\text{sample}}} \cdot c_{p,\text{ref}} \quad (1)$$

where m is the mass and ΔT the temperature rise on the rear surface. The reed sample has been coated with a graphite spray in order to enhance the absorption of the light pulse energy and the emission of IR radiation to the temperature detector, as well as to ensure the same emissivity and absorption coefficients for sample and reference. The accuracy of specific heat measure is 5–7 %. This allows the calculation of the thermal conductivity in the range of 0.1 – $2,000 \text{ W m}^{-1} \text{ K}^{-1}$ with an accuracy of 3–7 % for most materials.

Experimental Apparatus

The experimental apparatus (Fig. 1) consists of a tubular electric furnace (Nabertherm RT 50-250/11, inner diameter 50 mm; length: 360 mm; heated length: 250 mm), a

tubular quartz reactor (inner diameter: 20.5 mm; biomass seat length: 47.8 mm; thickness: 2.8 mm), a quartz condenser, a series of impinger bottles for the collection of tars and a module for gas sampling and measurement. The atmosphere inside the reactor is kept inert flowing nitrogen from a cylinder equipped with a pressure reducer. The gas produced inside the reactor flows through the condenser, where it is cooled. The tar collection is then performed in a series of six impinger bottles, according to the technical specification UNI CEN/TS 15439. In each test, small quantities (about 1.8 g) of ground reed (max size 1–2 mm) have been torrefied setting a temperature programme characterised by an initial ramp (heating rate of 28 or 50 °C min^{-1}) until the process temperature set up (280, 300 or 320 °C), that is then kept for 30 min. The nitrogen flow is set at 0.1 or $0.2 \text{ m}^3 \text{ h}^{-1}$, depending on the test run (Table 1). Each run has been repeated three times.

Torrefaction Kinetic Model

The above mentioned two-step kinetic mechanism applied by Prins [9, 10] to the weight mass loss of willow wood during torrefaction assumes that the original biomass (compound A) forms an intermediate product (compound B), whose degradation gives the final product (compound C) as char. In the proposed scheme (Fig. 2) the formation of volatiles (V_1 and V_2) products is assumed to take place through reactions in parallel to those giving the compounds B and C respectively. All the involved reactions are assumed to be of first order and the kinetic parameters are described by the usual Arrhenius equation:

$$k_i = k_{0,i} \exp\left(-\frac{E_{a,i}}{RT}\right) \quad i = 1, 2, V_1, V_2 \quad (2)$$

where $k_{0,i}$ is the pre-exponential factor, $E_{a,i}$ the activation energy, R the universal gas constant and T the temperature in Kelvin.

The experimental TG data (on dry basis) at temperature lower than 300 °C (corresponding to the upper limit for torrefaction) have been used to calibrate the model. More details about the global kinetic reactions scheme and the calibration method (i.e., least square optimization performed by means of a MatLab script) can be found in [27, 28].

Finite Volumes Thermofluidynamic Model

In order to assess the thermofluidynamics of the occurring process and to obtain an estimate of the reaction products, a numerical model based on a finite volumes method (f.v.m.) representation of the pilot system has been developed, suiting the commercial software ANSYS FLUENT [29].

Fig. 1 Set-up of the bench-scale batch pyrolysis/torrefaction system

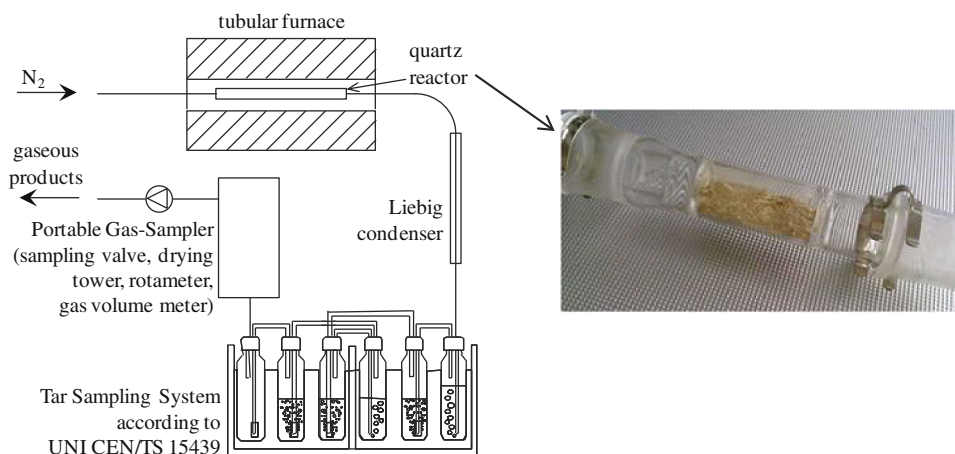


Table 1 Details of the experimental test runs

Parameter	Run 1	Run 2	Run 3	Run 4
N ₂ flow (m ³ h ⁻¹)	0.2	0.2	0.1	0.1
T _{max} (°C)	320	300	300	280
Heating rate (°C min ⁻¹)	28	28	50	50

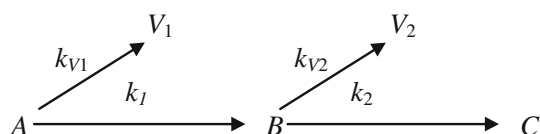


Fig. 2 Proposed torrefaction kinetic scheme

Implemented Equations

The numerical model integrates the mass, momentum and energy conservation equations within the oven and the reactor domains, respectively defined as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (3)$$

$$\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\bar{\tau}) + \rho \vec{g} + \vec{F} \quad (4)$$

$$\frac{\partial}{\partial t} (\rho E) + \nabla \cdot (\vec{v}(\rho E + p)) = \nabla \cdot (k_{eff} \nabla T + (\bar{\tau}_{eff} \cdot \vec{v})) + S_h \quad (5)$$

where the stress tensor and the total specific energy are respectively:

$$\bar{\tau} = \mu \left[\nabla \vec{v} + \frac{2}{3} \nabla \cdot \vec{v} I \right] \quad (6)$$

$$E = h - \frac{p}{\rho} + \frac{|\vec{v}|^2}{2}, \quad h = \int_{T_{ref}}^T c_p dT \quad (7)$$

and S_h is the heat source term. The subscript *eff* refers to the effective values of a variable or a parameter, including the

turbulent contribution. The turbulence model adopted is based on the Boussinesq's closure hypothesis, in particular implementing the realizable k - ϵ model [30] for the computation of the turbulent viscosity. With this approach the convective effect (amplified by the turbulent flow) due to the nitrogen flux inside the reactor has been taken into account.

The heat source term S_h has been introduced as a sink term (i.e., with values lower than zero), in order to take into account the heat required by the torrefaction process. Ohliger et al. [31] have found that the heat h_{tor} required for the torrefaction of lignocellulosic biomass (i.e., beech wood) with a residence time of 40 min and a torrefaction temperature varying between 270 and 300 °C is in the range 600–700 kJ kg⁻¹. This value accounts for the breakage of the bond between water and wood, the vaporisation of the moisture and the heat of reaction involved in the torrefaction process (integral heat of reaction).

Dimensionally, S_h is expressed in W m⁻³ and it is related to the heat required for torrefaction h_{tor} through the following equation:

$$h_{tor} = \int \frac{S_h}{\rho} dt \quad (8)$$

The S_h term has been described as a second order function of the temperature, and the parameter of the function has been treated as calibration parameters of the model, checking that the resulting h_{tor} is comparable to the one found by Ohliger et al.

Also the radiative exchange between the oven and the reactor surfaces have been implemented through the surface-to-surface (S2S) radiation model [32], in order to solve a completely coupled radiation, convection and conduction heat transfer problem.

Boundary and Subdomain Conditions

The assigned boundary conditions and subdomain materials are summarised in Fig. 3. The average inlet velocity has

been calculated starting from the nitrogen mass flow rate, kept constant during the experimental tests through a mass flow controller. The temperature of the oven surface has been measured through three K-type thermocouples placed along the longitudinal direction and set as boundary condition, while the temperatures detected in different points of the reactor (reactor wall, reactor inlet, reactor outlet and biomass bed) have been used for the calibration procedure. The aim of the calibration procedure is in fact to minimize the deviation between the measured temperature distribution and the simulated one.

The temperature program of the oven, consists of three stages: an initial heating ramp, a temperature plateau and a cooling stage. Initially the temperature increases with a fixed heating rate until the process temperature is reached. After that, the oven heaters are switched off and on in order to control the temperature and to keep it constant for 30 min, until the end of the heating process; during this stage the temperature at the centre of the oven is constant, whereas close to the extremity of the oven the heat losses becomes more and more relevant. Finally, the heaters are completely switched off until the oven is cooled at room temperature. The assigned temperature function at the oven wall has been simulated starting from the temperature measured in the middle section (T^*) and then considering a linear decreasing along the longitudinal direction:

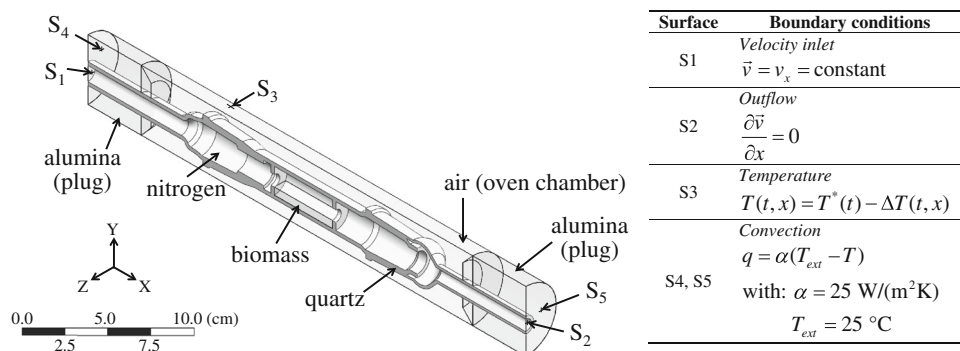
$$T(t, x) = T^*(t) - \Delta T(t, x) \quad (9)$$

ΔT is initially null until the maximum temperature is reached, at the end of the initial heating ramp. During the heating stage, on which the temperature T^* is kept constant at the center of the oven, the heat losses becomes more and more relevant, in particular close to the extremity of the oven. In order to take into account this effect, the ΔT term increases versus the distance from the center of the oven and versus the time, becoming equal to $c \cdot T^*$ at the oven extremity when the heating phase is concluded. The function $T = T(t, x)$ assigned as boundary condition at the oven wall is presented in Fig. 4, assuming c , one of the calibration parameters, equal to 0.2.

The modelled biomass volume is not subjected to variations along the time and takes up 3.6 cm^3 . It is as assuming that in the torrefaction range of temperatures the occurring thermal degradation does not lead to a significant change in the sample volume (i.e., only the porosity and then the density are subjected to variations) as a simplifying hypothesis. This hypothesis can be considered valid first of all because, due to the low temperatures involved in the torrefaction process, the gaseous products are released at pressure not high enough to broke the particles. In addition, the investigated reactor is a fixed bed one and because of the low biomass sample weight, low compression is applied by the superficial layers on the underlying particles. Under these conditions the biomass bed is hardly subjected to movements and friction (i.e., only the upper surface is subjected to friction due to the inert fluid flux) and it is therefore reasonable to expect that the single particles should keep approximately their size and shape varying only their porosity. This is also confirmed by visual observation of the biomass sample before and after the experimental runs.

Through the mass yield—predicted by the torrefaction model—it is then possible to estimate the function $\rho = \rho(T)$. In particular, the assumption of constant volume of the sample imply that the porosity and the density of the sample have a trend, respectively, similar and specular to the one of the mass loss. The thermal properties of reed determined through LFA—as well as the density value of 0.87 g cm^{-3} —refer to the compressed disk of reed powder used in the analysis, whose porosity can be assumed negligible. The experimental tests have been performed with a small quantity (about 1.8 g) of reed, ground in 1–2 mm pieces size. This corresponds, in the f.v.m. model, to an apparent density of about 0.5 g cm^{-3} and an equivalent porosity of approx. 43 %. In order to take this aspect into account, the reed thermal properties determined through LFA, as well as the density resulting from the mass loss (estimated through the torrefaction model calibrated vs TG data), have been averaged with the nitrogen properties, considering an equivalent porosity function $\phi = \phi(T)$:

Fig. 3 Boundary conditions and materials used in the finite volumes model



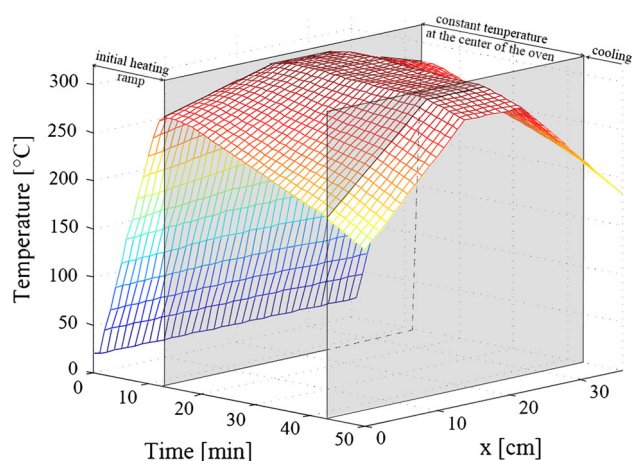


Fig. 4 Temperature function assigned as boundary condition at the oven wall

$$\rho_{exp.test}^{reed} = \phi \rho^{N_2} + (1 - \phi) \rho^{reed} \quad (10)$$

$$c_{p,exp.test}^{reed} = \phi c_p^{N_2} + (1 - \phi) c_{p,LFA}^{reed} \quad (11)$$

$$k_{exp.test}^{reed} = \phi k^{N_2} + (1 - \phi) k_{LFA}^{reed} \quad (12)$$

Two different implementations of the kinetic torrefaction model have been compared. In the first (simplified) approach the finite elements model has been used to estimate the temperature distribution inside the reactor during the experimental tests. An average (experimental) torrefaction temperature has been then calculated and used as input of the kinetic model. In the second approach the proposed kinetic scheme has been implemented directly in the f.v.m. model in order to predict the rate of the biomass decomposition. The results of the two models have been then compared with the experimental data.

Results and Discussion

Thermal Analysis and Torrefaction Model Calibration

Results of the torrefaction model calibration are reported in Fig. 5. The values of the model parameters that give the best fit of the experimental data are: 2.6×10^4 , 1.1×10^{10} , 3.2×10^7 and $1.6 \times 10^{10} \text{ s}^{-1}$ for $k_{0,1}$, $k_{0,2}$, $k_{0,V1}$ and $k_{0,V2}$ respectively, and 69,700, 150,000, 107,000 and 150,000 J mol^{-1} for $E_{a,1}$, $E_{a,2}$, $E_{a,V1}$ and $E_{a,V2}$ respectively. As it can be observed, the model fits with satisfying accuracy the experimental data at temperatures lower than 300 °C.

Assuming as simplifying hypothesis that in the torrefaction range of temperatures the occurring thermal degradation does not lead to a significant change in the sample volume (i.e., only the porosity and then the density are

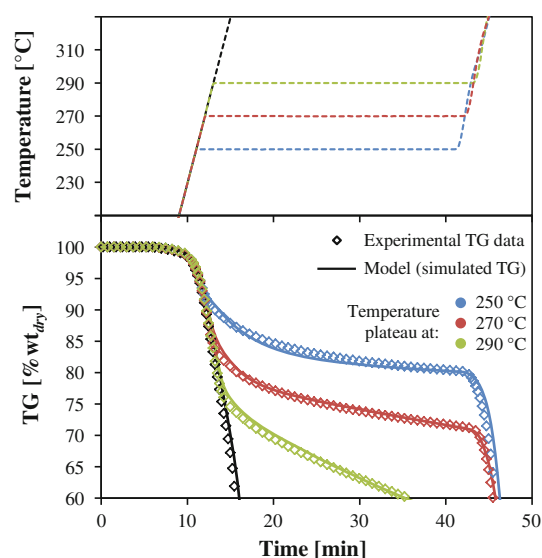


Fig. 5 Comparison between experimental TG data and values predicted by the torrefaction model

subjected to variations), it is possible to estimate the density variation, applying the calibrated torrefaction model. It is then possible to calculate the reed thermal conductivity knowing the thermal diffusivity and the specific heat:

$$k = \rho c_p \quad (13)$$

According to the torrefaction model, the density variation depends on the slope of the initial temperature ramp (i.e., the heating rate) and becomes significant at temperatures higher than 200 °C (Fig. 6).

The experimental values of thermal diffusivity and specific heat, measured through LFA until 175 °C, have been interpolated with the least square method using a third order polynomial function. The thermal properties have been then extrapolated in the range 175–300 °C (Fig. 7), obtaining c_p values between 1.9 and 2.9 $\text{J g}^{-1} \text{ K}^{-1}$, in good agreement with the data obtained in [31] for dry wood, that gives c_p values ranging from about 1.8 $\text{J g}^{-1} \text{ K}^{-1}$ at 180 °C to

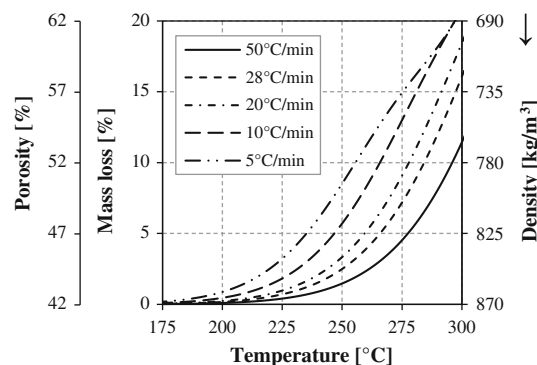


Fig. 6 Effect of the heating rate on mass loss, porosity and density according to the torrefaction model

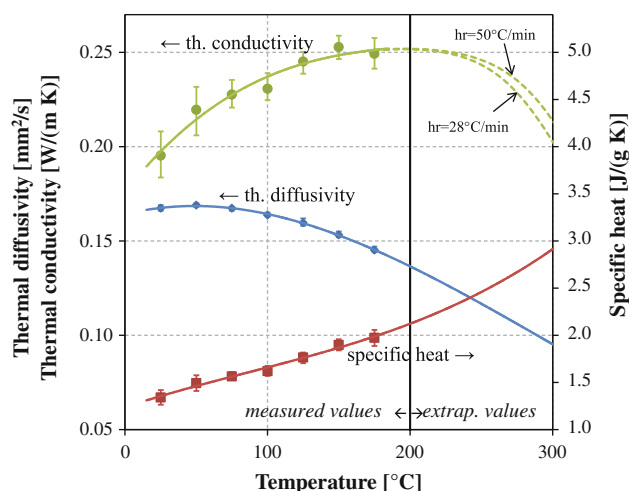


Fig. 7 Thermal diffusivity, specific heat and thermal conductivity of reed versus temperature; the values in the temperature range 25–175 °C at every 25 °C step are experimentally determined through LFA, the values at temperature higher than 200 °C are extrapolated taking into account (for the thermal conductivity) the effect of the temperature on the density

2.2 J g⁻¹ K⁻¹ at 260 °C. The effect of the heating rate on the density variation has been taken into account on the calculation of thermal conductivity values.

Fig. 8 Velocity profiles in different positions of the reactor (run 3)

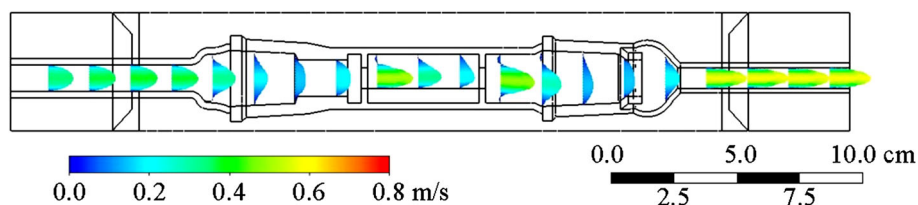
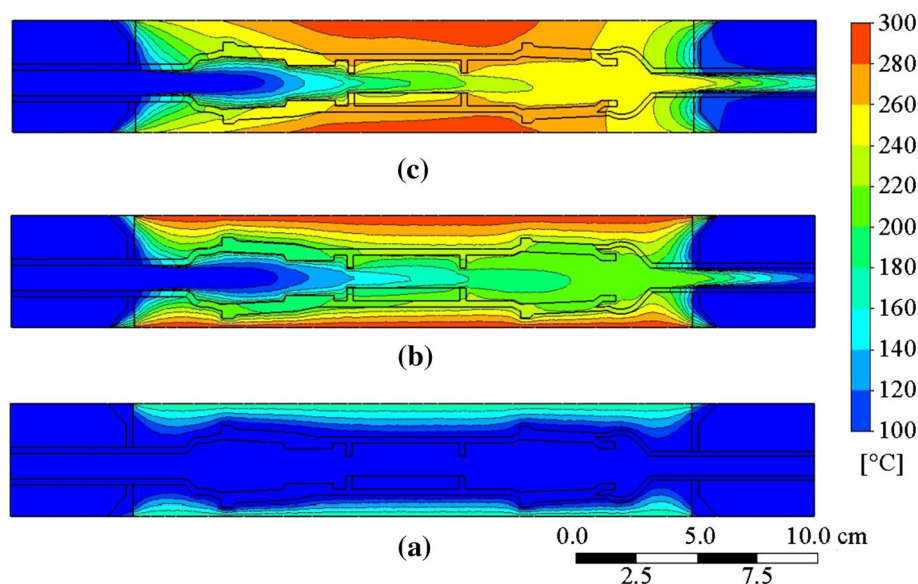


Fig. 9 Temperature distribution at different instants: **a** middle of the ramp, **b** top of the ramp and **c** end of the temperature program (run 2)



Finite Volumes Model

The function describing the heat source S_h has been calibrated and found to assume the following form between temperatures of the biomass bed in the range 25–300 °C, where the temperature is expressed in Kelvin:

$$S_h(T) = -1.425 T^2 + 5.420 \cdot 10^2 T - 4.611 \cdot 10^4 \quad (14)$$

As it can be expected, the function is negative and monotonically decreasing (increasing in absolute value) with the temperature, being the process globally endothermic. In fact, the function in this form takes into account the global heat of reaction (i.e., the heat required for drying the biomass, that is a very endothermic process, and the heat required by the torrefaction process).

Furthermore, the total heat consumption, calculated according to Eqs. 8 and 14, ranges from 645 kJ kg⁻¹ in run 1 to 611 kJ kg⁻¹ in run 4. This is in good agreement with the results obtained by Ohliger et al. [31] on torrefaction conditions.

Through the developed numerical model it is possible to estimate the velocity profiles and the temperature distribution inside the oven and the reactor at different time steps. Looking at the velocity profiles (Fig. 8), it is worth pointing out the presence of some areas of backflow in the

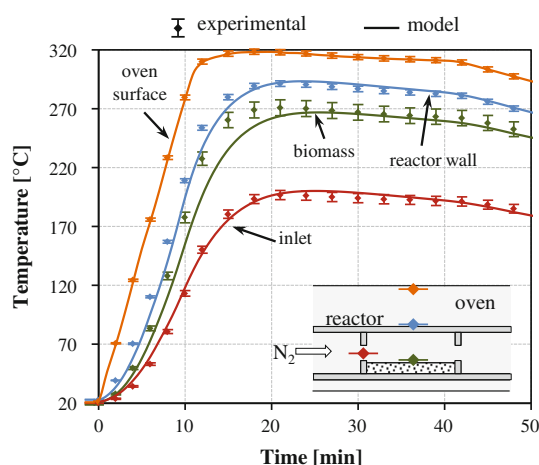


Fig. 10 Comparison between the temperature profiles measured in different positions of the oven and the reactor and the temperature profiles predicted through the finite volumes model (run 1)

Table 2 Experimental and predicted solid yield for the different test runs

Solid yield (%wt _{dry})	Run 1	Run 2	Run 3	Run 4
Experimental	67.5 ± 1.3	75.7 ± 2.1	69.8 ± 5.0	77.9 ± 1.2
Model	67.0	76.1	70.3	77.9
Deviation	0.74 %	0.53 %	0.72 %	0.01 %

reactor, related to the turbulent flow generated by the narrow gaps where the biomass is placed. The turbulent flow of the nitrogen flux entering in the reactor has a strong effect on the temperature distribution, as it can be clearly observed in Fig. 9.

Through the numerical simulation it is also possible to extract the temperature profiles versus time in different points of the domains. The predicted temperature profiles (Fig. 10) show good agreement with the measured ones, making exception for the temperature ramp (approx. 10 % deviation in the ramp, approx. 2.5 % deviation in the temperature plateau).

Due to the relatively low torrefaction temperatures, the variability of the temperature distribution inside the biomass volume is limited. For example, making reference to run 2 and looking at the statistics of the temperature distribution in the biomass volume at each time step, the standard deviation reaches the maximum value of 11.2 °C at the top of the heating ramp, decreasing to 10.4 °C in the constant temperature stage. As a consequence, the two different implementations of the kinetic model (i.e., making reference to the average or to the local temperature) do not show significant deviations (the difference between the predicted mass yields is lower than 1 % in each run).

It is worth to point out that, although the high number of involved parameters (i.e., thermal properties of the different materials) and the simplifying hypothesis, the results of the model describing the mass yield of the torrefaction runs are characterised by a satisfying agreement with the experimental data, as shown in Table 2.

Conclusions

A numerical torrefaction model for common reed (*P. australis*) has been developed and validated. In order to predict the rate of the biomass decomposition (i.e., yield of the reaction products) and characterise the thermo-fluid-dynamics of the reactor, a heat, mass and momentum transfer model based on a finite volumes method (f.v.m.) representation has been developed and supplemented with a torrefaction kinetic model, consisting of a two-step scheme previously proposed. The kinetic routine has been calibrated utilizing the results of thermogravimetric analysis (TGA), whereas the complete (i.e., physical–chemical) model has been validated using the experimental data obtained through a bench-scale batch reactor for torrefaction, varying the main process parameters.

The results of the proposed model fit with satisfying accuracy the experimental data and they are quite encouraging, in particular considering the complexity of the simulated geometry. Thus, the proposed modelling approach seems to be a suitable tool for the simulation of a torrefaction reactor and useful for the optimization of such kind of systems.

References

1. Pentananunt, R., Rahman, A.N.M.M., Bhattacharya, S.C.: Upgrading of biomass by means of torrefaction. *Energy* **15**, 1175–1179 (1990)
2. Lipinsky, E.S., Arcate, J.R., Reed, T.B.: Enhanced wood fuels via torrefaction. *Fuel Chem. Div. Prepr.* **47**, 408–410 (2002)
3. Arias, B., Pevida, C., Fermoso, J., Plaza, M.G., Rubiera, F., Pis, J.J.: Influence of torrefaction on the grindability and reactivity of woody biomass. *Fuel Process. Technol.* **89**, 169–175 (2008)
4. Bridgeman, T.G., Jones, J.M., Shield, I., Williams, P.T.: Torrefaction of reed canary grass, wheat straw and willow to enhance solid fuel qualities and combustion properties. *Fuel* **87**, 844–856 (2008)
5. Bridgeman, T.G., Jones, J.M., Williams, A., Waldron, D.J.: An investigation of the grindability of two torrefied energy crops. *Fuel* **89**, 3911–3918 (2010)
6. Repellin, V., Govin, A., Rolland, M., Guyonnet, R.: Energy requirement for fine grinding of torrefied wood. *Biomass Bioenergy* **34**, 923–930 (2010)
7. Prins, M.J., Ptasiński, K.J., Janssen, F.J.J.G.: More efficient biomass gasification via torrefaction. *Energy* **31**, 3458–3470 (2006)

8. Di Blasi, C., Lanzetta, M.: Intrinsic kinetics of isothermal xylan degradation in inert atmosphere. *J. Anal. Appl. Pyrolysis*. **40–41**, 287–303 (1997)
9. Prins, M.J., Ptasiński, K.J., Janssen, F.J.J.G.: Torrefaction of wood part 1. Weight loss kinetics. *J. Anal. Appl. Pyrolysis*. **77**, 28–34 (2006)
10. Prins, M.J.: Thermodynamic analysis of biomass gasification and torrefaction. Technische Universiteit Eindhoven, Eindhoven, the Netherlands (2005)
11. Rousset, P., Turner, I., Donnot, A., Perré, P.: The choice of a low-temperature pyrolysis model at the microscopic level for use in a macroscopic formulation. *Ann. For. Sci.* **63**, 213–229 (2006)
12. Broido, A., Evett, M., Hodges, C.C.: Yield of 1,6-anhydro-3,4-dideoxy- β -D-glycero-hex-3-enopyranos-2-ulose (levoglucosenone) on the acid-catalyzed pyrolysis of cellulose and 1,6-anhydro- β -D-glucopyranose (levoglucosan). *Carbohydr. Res.* **44**, 267–274 (1975)
13. Bradbury, A.G.W., Sakai, Y., Shafizadeh, F.: A kinetic model for pyrolysis of cellulose. *J. Appl. Polym. Sci.* **23**, 3271–3280 (1979)
14. Van der Stelt, M.J.C., Gerhauser, H., Kiel, J.H.A., Ptasiński, K.J.: Biomass upgrading by torrefaction for the production of biofuels: a review. *Biomass Bioenergy*. **35**, 3748–3762 (2011)
15. Ratte, J., Fardet, E., Mateos, D., Héry, J.-S.: Mathematical modelling of a continuous biomass torrefaction reactor: TOR-SPYDTM column. *Biomass Bioenergy*. **35**, 3481–3495 (2011)
16. Shafizadeh, F., Chin, P.P.S.: Thermal deterioration of wood. In: Goldstein, I.S. (ed.) *Wood Technology: Chemical Aspects*, pp. 57–81. American Chemical Society, Washington, D.C. (1977)
17. Whitaker, S.: Simultaneous heat, mass, and momentum transfer in porous media: a theory of drying. *Adv. Heat Transf.* **13**, 119–203 (1977)
18. Ratte, J., Marias, F., Vaxelaire, J., Bernada, P.: Mathematical modelling of slow pyrolysis of a particle of treated wood waste. *J. Hazard. Mater.* **170**, 1023–1040 (2009)
19. Di Blasi, C.: Modeling chemical and physical processes of wood and biomass pyrolysis. *Prog. Energy Combust. Sci.* **34**, 47–90 (2008)
20. Hankalin, V., Ahonen, T., Raiko, R.: On thermal properties of a pyrolysing wood particle. Finnish-Swedish Flame Days 2009, p. 16. Naantali, Finland (2009)
21. Strezov, V., Evans, T.J., Hayman, C.: Thermal conversion of elephant grass (*Pennisetum purpureum Schum*) to bio-gas, bio-oil and charcoal. *Bioresour. Technol.* **99**, 8394–8399 (2008)
22. Bonanno, G., Lo Giudice, R.: Heavy metal bioaccumulation by the organs of *Phragmites australis* (common reed) and their potential use as contamination indicators. *Ecol. Indic.* **10**, 639–645 (2010)
23. Patuzzi, F., Mimmo, T., Cesco, S., Gasparella, A., Baratieri, M.: Common reeds (*Phragmites australis*) as sustainable energy source: experimental and modelling analysis of torrefaction and pyrolysis processes. *GCB Bioenergy*. (2012). doi:[10.1111/gcbb.12000](https://doi.org/10.1111/gcbb.12000)
24. Bragato, C., Brix, H., Malagoli, M.: Accumulation of nutrients and heavy metals in *Phragmites australis* (Cav.) Trin. ex Steudel and *Bolboschoenus maritimus* (L.) Palla in a constructed wetland of the Venice lagoon watershed. *Environ. Pollut.* **144**, 967–975 (2006)
25. Cowan, R.D.: Proposed method of measuring thermal diffusivity at high temperatures. *J. Appl. Phys.* **32**, 1363 (1961)
26. Cowan, R.D.: Pulse method of measuring thermal diffusivity at high temperatures. *J. Appl. Phys.* **34**, 926 (1963)
27. Baratieri, M., Patuzzi, F., Thevs, N., Zerbe, S.: Assessment of suitable energy conversion scenarios of common reeds, *Phragmites australis*. In: ETA Florence (ed.) 19th European Biomass Conference & Exhibition, pp. 1501–1514. Berlin, Germany (2011)
28. Patuzzi, F., Baratieri, M.: Multistage modeling and experimental design for the assessment of suitable energy conversion scenarios of wetland biomass. 66^o Congresso ATI., Rende, Cosenza, Italy (2011)
29. ANSYS FLUENT Theory Guide. (2011)
30. Shih, T.-H., Liou, W.W., Shabbir, A., Yang, Z., Zhu, J.: New k- ϵ eddy-viscosity model for high Reynolds number turbulent flows—model development and validation. *Comput. Fluids* **24**, 227–238 (1995)
31. Ohliger, A., Förster, M., Kneer, R.: Torrefaction of beechwood: a parametric study including heat of reaction and grindability. *Fuel* **104**, 607–613 (2013)
32. Siegel, R., Howell, J.R.: Thermal Radiation Heat Transfer. Hemisphere Publishing Corporation, Washington, D.C (1992)